IUCLID 5
Guidance and Support

Installation Guide for IUCLID 5.5 Standalone Application

Custom Installation on Microsoft® Windows®

March 2013

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Chapter 1. Introduction

IUCLID 5 can be installed either as a stand-alone application, or in a multi-user environment that uses client-server architecture. The purpose of this document is to describe how to install manually, a single stand-alone application version of the IUCLID 5 software onto a computer running Microsoft® Windows® (hereafter referred to as Windows). The installation is performed by ensuring that prerequisite software is installed, copying files to the computer and then, if necessary, making some configuration changes that are explained in this document. If the instructions in this document are followed exactly, no prior specialist knowledge is required of either the IUCLID 5 software, or the software components required to run it.

The stand-alone installation of IUCLID 5 should be carried out manually if you want to use a database and version of Java other than those that are used with the IUCLID 5 installer for Windows. For example, the database Oracle rather than PostgreSQL.

If you encounter any problems during the installation that cannot be solved using information in this manual, or the documentation of third party softwares; before contacting ECHA Helpdesk, please try the IUCLID FAQ located at the IUCLID web site http://iuclid.eu.

1.1. Hardware requirements

The following requirements are provided as only a guide.

- At least 2 GB of RAM on the mother board; 4 GB if PostgreSQL is run on the same machine as IUCLID 5
- Intel Pentium Dual @ 1.8 GHz
- 10 GB of hard-drive space

An installation of IUCLID 5 will most likely run on a lower specified machine but the performance might not be satisfactory. The requirements depend in part on the version of Windows and the IUCLID 5 plugins that are in use. For example, using the Query Tool plugin will increase the resources required to obtain a reasonable running speed; especially on a large database. The handling of large attachments increases the memory requirement.

1.2. Software requirements

The software prerequisites for the installation are as follows:

- Windows preferably with knowledge of the administrator password.

  It is recommended to carry out the installation from a standard type of Windows user account, rather than an administrator. You will be prompted to enter the administrator password where necessary.

- Java SE - Runtime Environment 7. IUCLID 5.5.0 is compatible with Java 6, but the vendor, Oracle, recommends to uninstall Java SE 6, and then to install the latest update of Java 7. Various scenarios involving the use of IUCLID 5, Java 6 and Java 7 can be found in the IUCLID FAQ located at the IUCLID web site http://iuclid.eu.

- Database - PostgreSQL 8.4 and 9.0 are supported, but 9.0 is recommended; or Oracle 10g or higher. IUCLID 5 works with both PostgreSQL **and** Oracle, therefore you need to chose which database to use, and then use only that. You do not need to install both PostgreSQL **and** Oracle.

  The Oracle driver for Java is no longer supplied with the IUCLID 5 installation package. The correct driver for the combination of Java and Oracle versions in use must be obtained from the Oracle web site and installed in the appropriate folder. The most recent driver for your version of Oracle should work. For example, for Oracle 11g Release 2 (11.2.0.2.0), the name of the driver is `ojdbc6.jar`. For use with Tomcat, the driver must be placed in Tomcat's library folder, e.g. `Tomcat\lib`.

- A package for the installation of a standalone (workstation) version of IUCLID 5 can be downloaded without charge from the IUCLID web site.
- Once you have completed the installation of IUCLID 5, you should test it by starting and configuring it. The configuration requires access to at least a legal entity file (LEOX). The creation of a LEOX is described on the IUCLID web site where the installation software is published. In addition, it is recommended to upload a set of reference substances and the EC inventory. These are also available from the web site at which the IUCLID 5 software is published.

Tip

Time and IT resources can be saved by importing into IUCLID 5 only the Reference substances you need. Various different sizes of Reference substance inventory can be downloaded from the IUCLID web site. There is a *full set,* a *reduced list*, and a function that allows you to create your own inventory using common identifiers as selection criteria, such as EC Number, and IUPAC name. Before importing the *full set*, consider carefully whether it is really necessary. Reference substances that are not imported during the initialisation process can be imported later. A simple compromise is to start with the *reduced list*.

For more information regarding system requirements, see the FAQ on the IUCLID web site located at http://iuclid.eu.

Chapter 2. Making a fresh installation of IUCLID 5

If Java and PostgreSQL are already installed, go straight to Section 2.1.3, “Configuration of PostgreSQL”.

2.1. Installation of the Software Required by IUCLID 5

The installation of third party software is described by the respective publishers. Please refer to their web sites for full instructions.

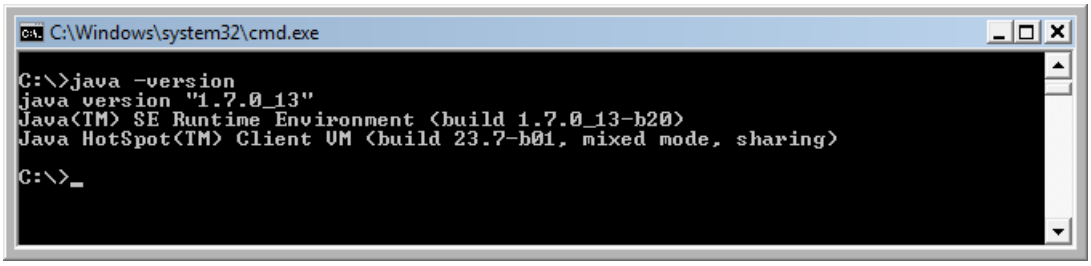
2.1.1. Installation of Java

1. Verify whether Java (JRE) of the correct version is installed on the computer to which IUCLID 5 will be installed:

   Open a command prompt (Start -> Run… -> Open: cmd). At the command prompt, enter the following:

   ```
   java -version
   ```

   Figure 2.1. Check version of Java

2. If a message similar to the one shown in the screen shot above is not shown, the system does not have Java SE installed, in which case, download the latest update of Java SE 7 (JRE) from the vendor's site http://www.oracle.com, and then install it. If the version is "1.6.x", the default version of Windows is Java SE 6 (JRE). IUCLID 5.5.0 is compatible with Java 6, but the vendor, Oracle, recommends to uninstall Java SE 6, and then to install the latest update of Java 7. Information relevant to the version of Java used with IUCLID 5 can be found in the IUCLID FAQ located at the IUCLID web site http://iuclid.eu.

   The installation process is illustrated in some example screen shots below.

Figure 2.2. Select either the default, or a custom destination for the installation

Java Setup - Welcome
Java
ORACLE
Welcome to Java
Java provides safe and secure access to the world of amazing Java content. From business solutions to helpful utilities and entertainment, Java makes your internet experience come to life.
Note: No personal information is gathered as part of our install process.
Click here for more information on what we do collect.
Click Install to accept the license agreement and install Java now.
Change destination folder
Cancel
Install >

Figure 2.3. Installation is under way

Java Setup - Progress
Java
ORACLE
Status: Installing Java
3 Billion Devices Run Java
Computers, Printers, Routers, Cell Phones, BlackBerry, Kindle, Parking Meters, Public Transportation Passes, ATMs, Credit Cards, Home Security Systems, Cable Boxes, TVs...
ORACLE

Figure 2.4. Installation of Java is complete

Java Setup - Complete
Java
ORACLE
You have successfully installed Java
When Java updates are available, you will be prompted to download and install. We recommend you always do so to ensure your system has the latest performance and security improvements.
See the instructions if you want to change this behavior.
Close

2.1.2. Installation of PostgreSQL

If either version 8.4 or 9.0 of PostgreSQL are already installed and running as a service with a user `postgres`, the existing installation can be used. Later versions of PostgreSQL might work, but they are not yet supported. If PostgreSQL is not already installed on the computer, or you would like to upgrade it, download the new version of PostgreSQL from the site *www.postgresql.org/download* and install it. The web site of PostgreSQL offers a range of alternative ways to download and install the PostgreSQL software. The screen shots shown below show the use of the *one click installer*. An example of the file name of the installer is *postgresql-9.0.12-2-windows-x64.exe*.

The default fresh installation of PostgreSQL, made using the *one click installer*, automatically starts PostgreSQL as a service, creates the user `postgres` if necessary, and supplies administration tools (e.g. pgAdmin III) that can be used to manage databases. If the installer creates the database superuser `postgres`, you will have to enter a password for it into step 4 of the *one click installer*, as shown in the sequence of figures below. Remember this password because it will be required later, during the configuration of IUCLID 5. If you are unsure of what values to enter into the *one click installer*, use the pre-filled defaults.

Figure 2.5. Installer for PostgreSQL

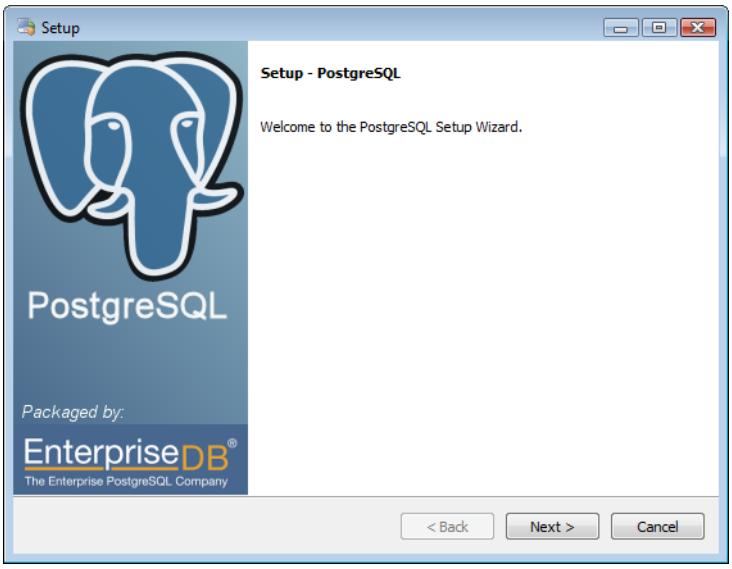


Figure 2.6. Installation directory for PostgreSQL

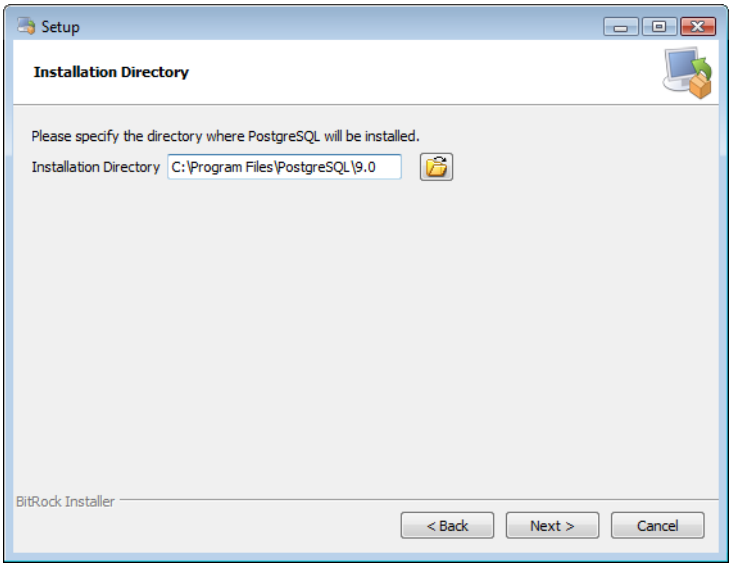


Figure 2.7. Data directory for PostgreSQL

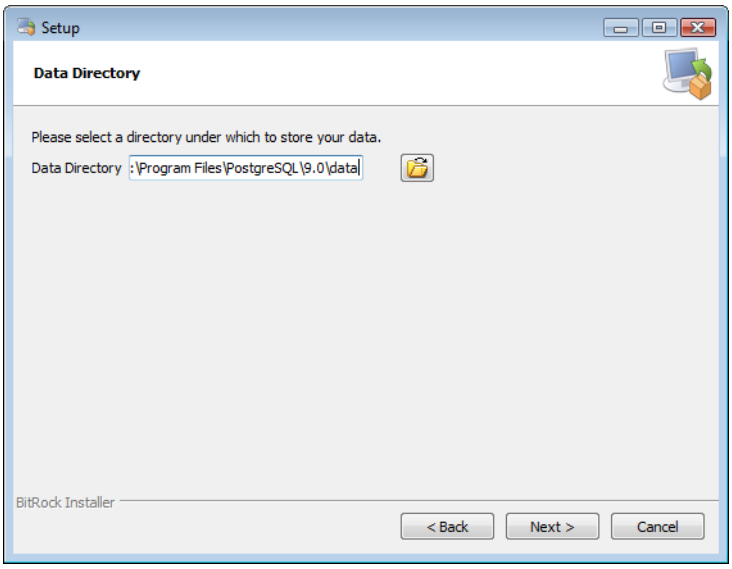


Figure 2.8. Password for the database superuser (postgres) and the Windows service account (postgres)

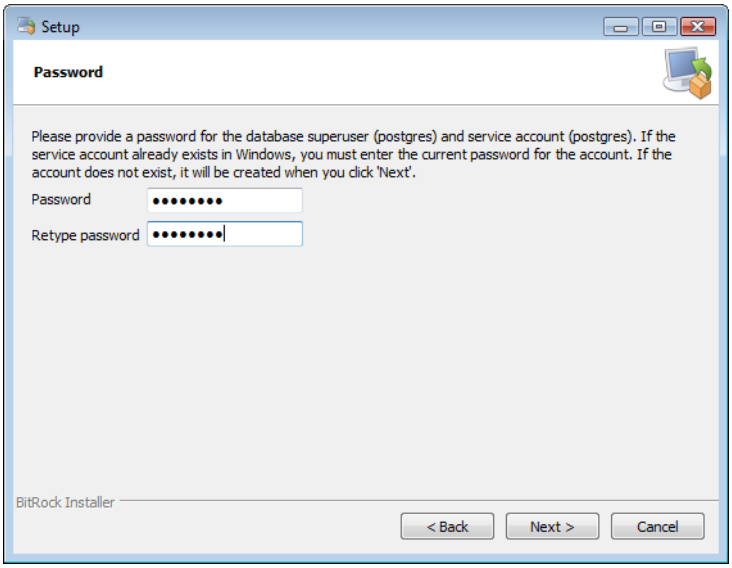

Setup
Password
Please provide a password for the database superuser (postgres) and service account (postgres). If the service account already exists in Windows, you must enter the current password for the account. If the account does not exist, it will be created when you click 'Next'.
Password
Retype password
BitRock Installer
< Back
Next >
Cancel

Figure 2.9. Port number for PostgreSQL

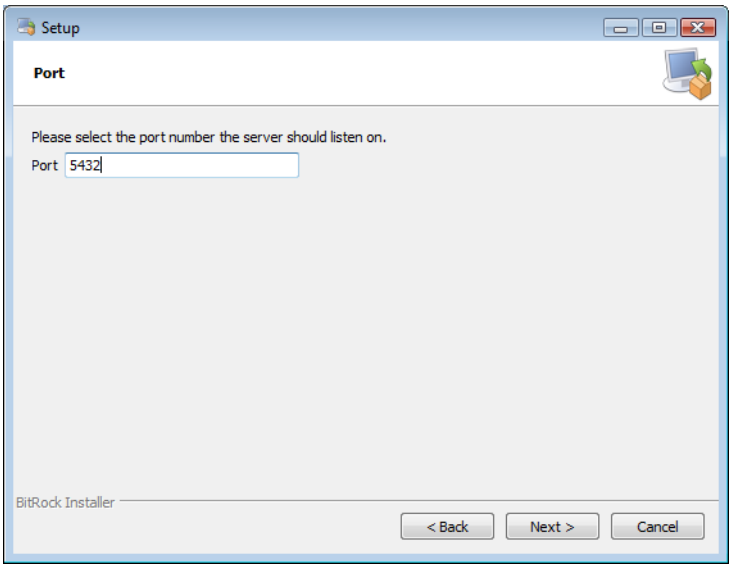


Figure 2.10. Set the default locale for PostgreSQL

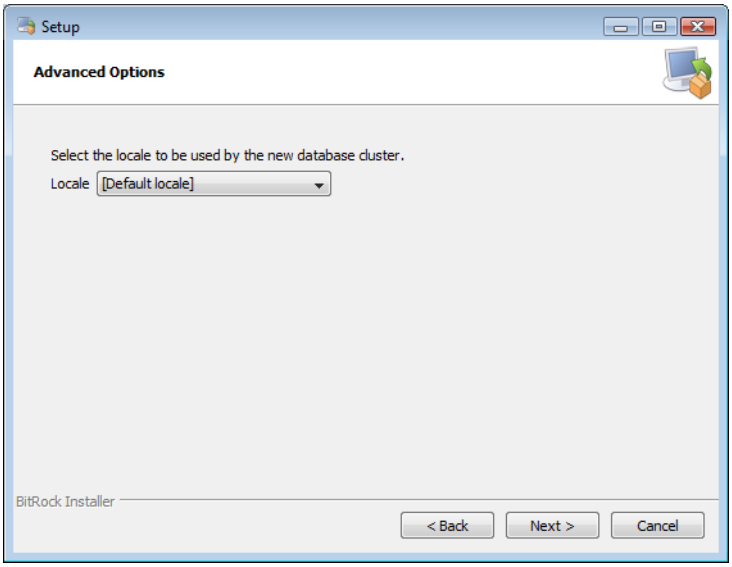


Figure 2.11. Confirm installation of PostgreSQL

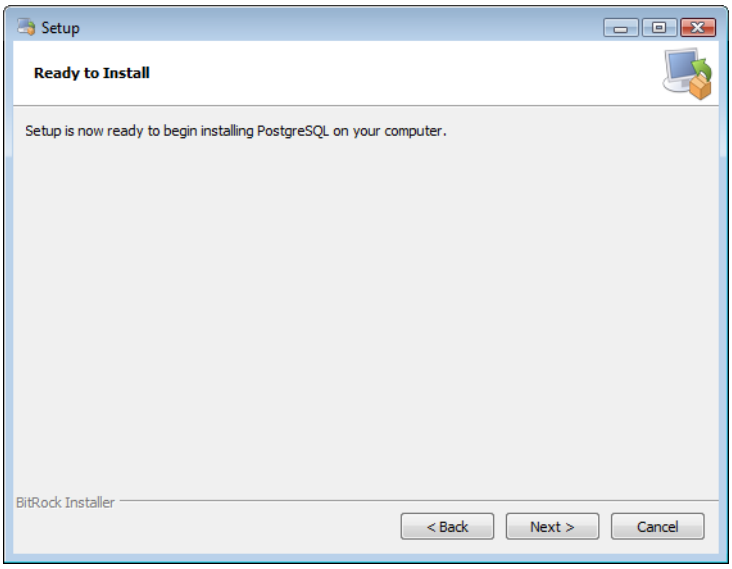


Figure 2.12. Installation of PostgreSQL in progress

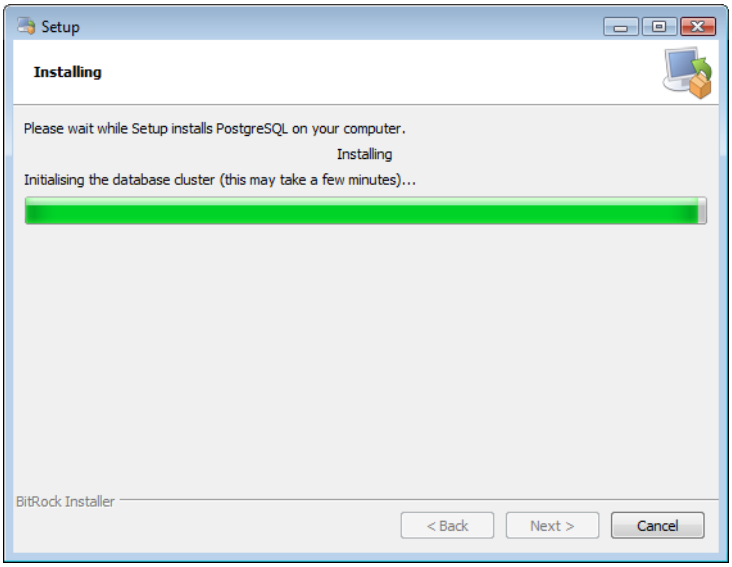


Figure 2.13. Installation of PostgreSQL complete

Setup
Completing the PostgreSQL Setup Wizard
Setup has finished installing PostgreSQL on your computer.
Launch Stack Builder at exit?
Stack Builder may be used to download and install additional tools, drivers and applications to complement your PostgreSQL installation.
PostgreSQL
Packaged by:
EnterpriseDB
The Enterprise PostgreSQL Company
< Back
Finish
Cancel

Unless you particularly want to run the Stack Builder, untick the box in the screen shown above. To finish the installation, click on the button Finish.

2.1.3. Configuration of PostgreSQL

A new user and a new database need to be created.

Tip

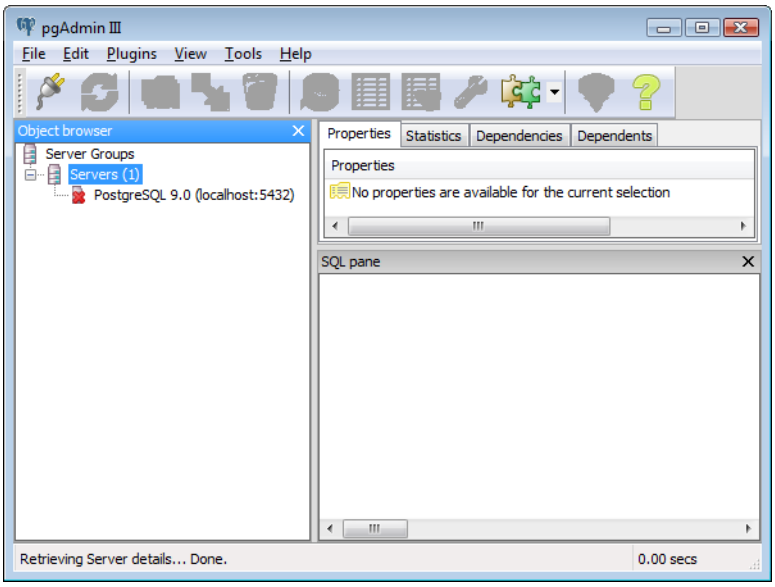
IUCLID 5 is configured by default to connect to the database using username:*iuclid5* and password:*iuclid5*. It is convenient to specify the same password now, and change it later when the application is set up correctly.

Important

Take note of the password of this user. This user name and password will be needed later to connect IUCLID 5 to the database.

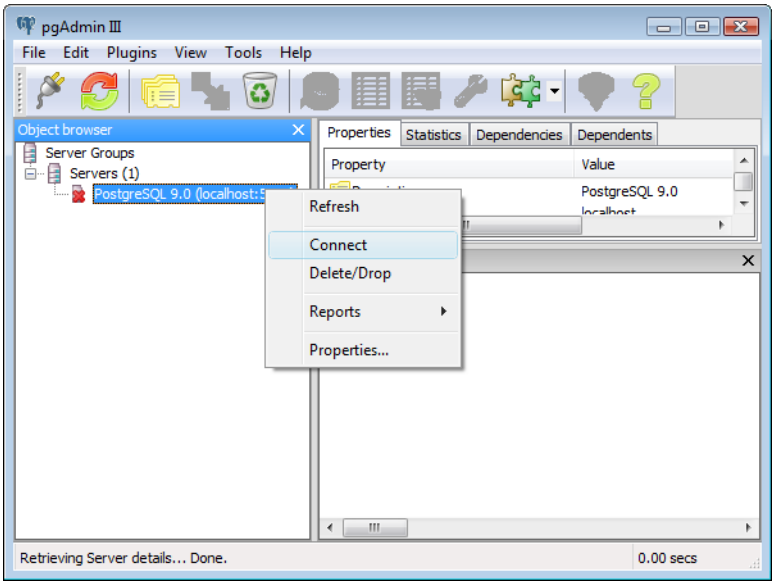
The program pgAdmin III can be used to create the database as follows. Start pgAdmin III from the menu *Start / All Programs / PostgreSQL9.0*. After the splash screen has appeared and you have closed the pop-up window that shows usage tips, the following screen is shown.

Figure 2.14. pgAdmin III interface on first opening



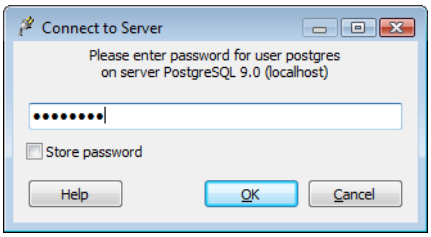
Right-click the text *PostgreSQL 9.0 (localhost:5432)* that is under the word *Servers* highlighted in blue in the figure above. Select *connect* as shown below.

Figure 2.15. Connect pgAdmin III to PostgreSQL as user postgres



Enter the password for user *postgres* as given in the postgres installer Figure 2.8, “Password for the database superuser (postgres) and the Windows service account (postgres)” then click *OK*. It is recommended to store the password to facilitate future access.

Figure 2.16. Authenticate the user postgres



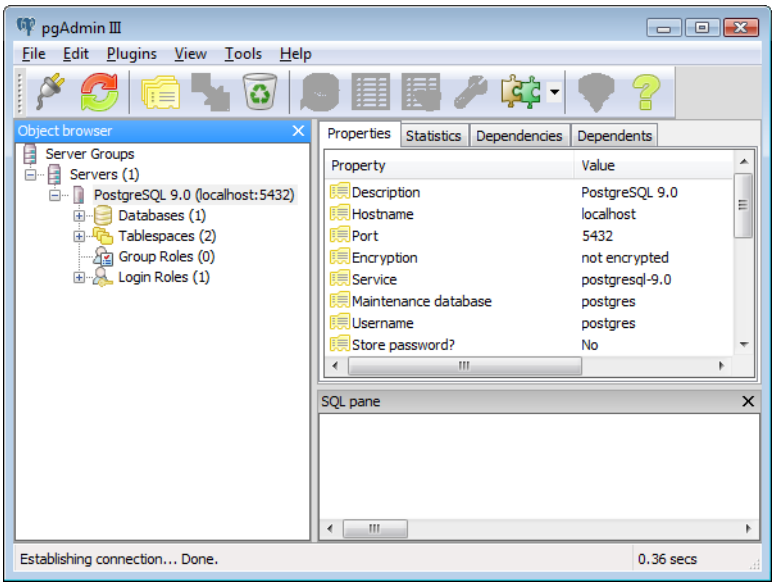
If you elect to save the password, the following warning might be displayed. Click *OK*

Figure 2.17. Saving passwords Warning

Guru Hint - Saving passwords
Saving passwords
WARNING: You have opted to save your password. It will be stored in plain text in your home directory on *nix systems, or in your user profile on Windows. If you do not want this to happen, please press the Cancel button.
pgAdmin uses PostgreSQL's 'pgpass' mechanism to store your passwords. On *nix systems, the password will be stored in ~/.pgpass, whilst on Windows systems it will be stored in %APPDATA%\PostgreSQL\pgpass.conf (%APPDATA% is the 'Application Data' folder in your user profile). This mechanism is used by default by all programs that use the libpq library to access the server, which includes command line applications such as pg_dump and pg_restore, other GUI applications, and drivers such as psqlODBC. This means that those applications may automatically connect to the server using your stored password. If you do not want this to happen, you should not use the Store Password option in pgAdmin.
Do not show this hint again
Help
OK
Cancel

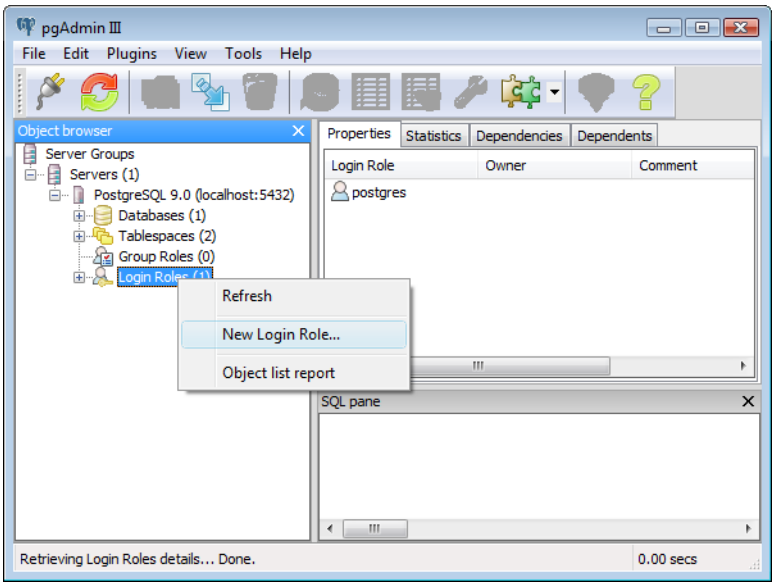
Expand the tree for *PostgreSQL 9.0 (localhost:5432)* by clicking the plus sign that has just appeared next to it, as shown in the figure below.

Figure 2.18. Initial screen in pgAdmin III



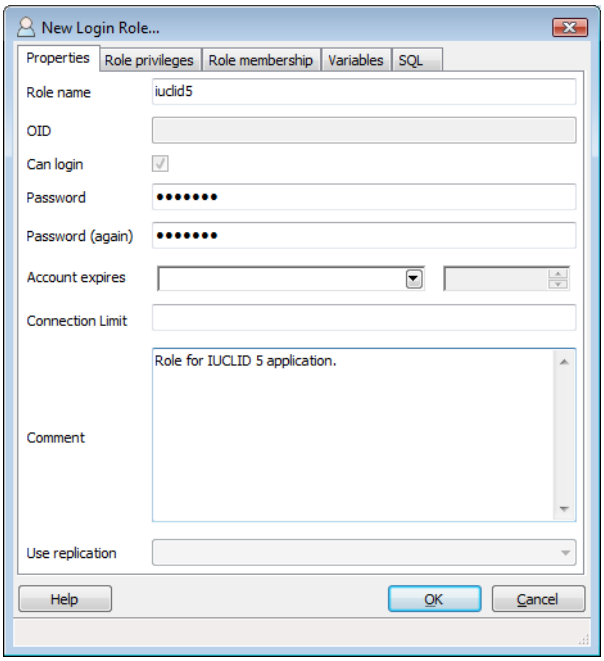
Right-click on *Login Roles* and select *New Login Role...*.

Figure 2.19. Select the option New Login Role



Enter the name of the login role. We recommend using a name of `iuclid5`.

Figure 2.20. Create a new login role (i.e. a user) with the name iuclid5



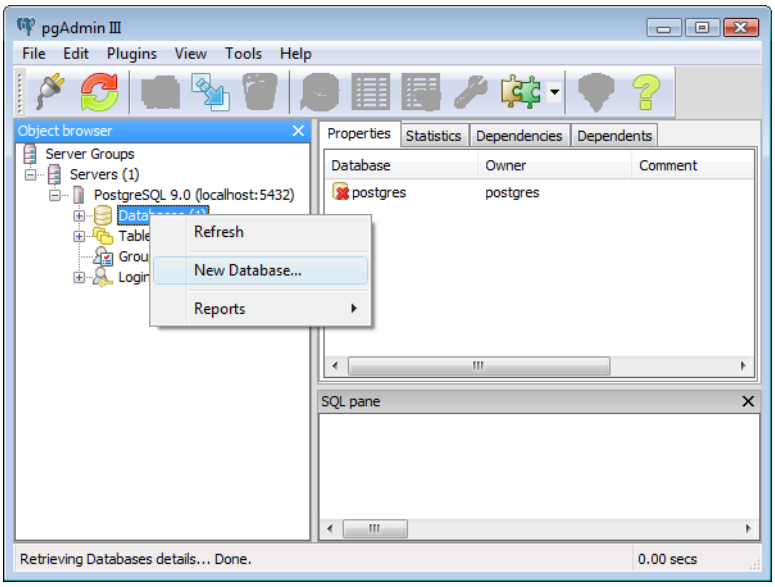
The login role can have a password set, although this is optional.

Important

Make a note of the user name and if set, the password. They are referred to later in the installation, in Section 2.3.1, “Database connection for PostgreSQL”. We recommend using `iuclid5` as the name of the login role, and for the value of the password.

Request a new database by right-clicking the item *Databases*, and selecting *New Database...* as shown in the figure below.

Figure 2.21. Request a new database in pgAdmin III

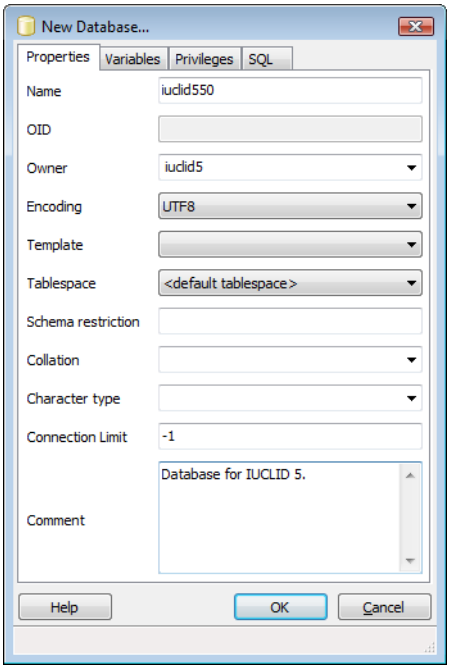


Enter the database name and owner. We recommend using a name of `iuclid` followed by the version number, for example `iuclid550`. Select the owner to be the value used in the previous step, e.g. `iuclid5`. The encoding must be left at the default value of UTF8. Click *OK*.

Important

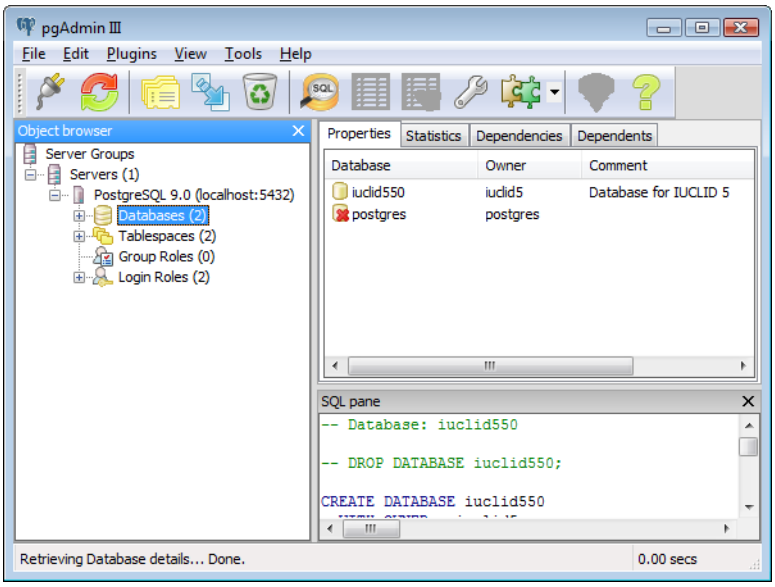
Make a note of the database name. It is referred to later in the installation, in Section 2.3.1, “Database connection for PostgreSQL”.

Figure 2.22. Enter the details of IUCLID 5's database into pgAdmin III



As you can see from the figure below, there is now a new database named *iuclid550*.

Figure 2.23. List of databases in pgAdmin III



You can now close *pgAdmin III* and move directly to the installation of IUCLID 5.

2.1.4. Installation and Configuration of Oracle

The installation and configuration of an Oracle database are out of the scope of this document. For full details, consult the documentation supplied by the vendor. Information specific to IUCLID is given in the IUCLID installation manual, *Client-Server Architecture (Oracle®)*, which is available from the same site as this manual.

The configuration of the connection between an Oracle database and IUCLID 5 is described later in this document in Section 2.3.2, “Database connection for Oracle”.

2.2. Installing IUCLID 5

Unzip the archive that contains the software for the manual installation of IUCLID 5. Do not unzip or change the relative location of any of the plugin archives. Create an installation directory for IUCLID 5 somewhere convenient (for example `C:\Program Files\IUCLID5`). Copy the directory `workstation` and all its contents into the installation directory.

2.3. Post-installation configuration

If you are making a fresh installation of IUCLID 5, using PostgreSQL for the database, and only the default values suggested in this document, IUCLID 5 should start without any additional configuration. Otherwise, it is necessary to set values for parameters in the file `workstation.properties`, that is located in a folder named `conf` within the installation folder. Values set in the file over-ride hard-coded defaults. Parameters for which you do not want to set your own values should be commented out by placing the symbol # at the start of the line. The meanings of the parameters and their default configurations are described in the sub-sections below.

Tip

If you experience difficulties in saving changes to the properties file, try granting write access for it, to standard local users. This can be done by right-clicking on the file, selecting *properties / security*,

highlighting your user group or user name, then ticking the box *allow* for *write*. You will need to supply an administrator password. The *write* permission can be revoked after your IUCLID 5 has been successfully configured.

2.3.1. Database connection for PostgreSQL

This is where the values used to connect IUCLID 5 to a PostgreSQL database are defined. Usually, only the first three values need to be considered. These define the name of the database, the login role (username) and its password, as shown below.

```
# ---------------------------
# Settings for using PostgreSQL
# ---------------------------
hibernate.connection.url=jdbc:postgresql://localhost:5432/<database>
hibernate.connection.username=<username>
hibernate.connection.password=<password>
hibernate.connection.driver_class=org.postgresql.Driver
hibernate.dialect=org.hibernate.dialect.PostgreSQLDialect
```

The default values are shown below.

```
# ---------------------------
# Settings for using PostgreSQL
# ---------------------------
hibernate.connection.url=jdbc:postgresql://localhost:5432/iuclid550
hibernate.connection.username=iuclid5
hibernate.connection.password=iuclid5
hibernate.connection.driver_class=org.postgresql.Driver
hibernate.dialect=org.hibernate.dialect.PostgreSQLDialect
```

2.3.2. Database connection for Oracle

This is where the values used to connect IUCLID 5 to an Oracle database are defined. The default values are shown below. Uncomment the lines as required.

```
# ---------------------------
# Settings for using ORACLE 10g
# ---------------------------
#hibernate.connection.username=<username>
#hibernate.connection.password=<password>
#hibernate.connection.driver_class=oracle.jdbc.driver.OracleDriver
#hibernate.connection.url=jdbc:oracle:thin:@localhost:1521:<database>
#hibernate.hbm2ddl.auto=validate
#hibernate.dialect=eu.eca.iuclid.server.system.persistence.ExtendedOracle9Dialect
#hibernate.jdbc.use_streams_for_binary=false
```

2.3.3. Window title

It is possible to define a name that is displayed at the top left of the IUCLID 5 interface. Enter the name into the value of the parameter shown below. The default value is shown below. Uncomment the line as required.

```
# ---------------------------
# configurable default window title
# overrides the title defined in the source code
# ---------------------------
#connection.client.window.title=IUCLID 5.5.0
```

2.3.4. Security settings for user accounts

IUCLID 5 has features designed to control the level of security of authentication of user accounts. The level of security can be tailored to that required for the particular installation of IUCLID 5. For example, when setting passwords for their user accounts, users can be forced to enter values that have a minimum strength. The values of the parameters that determine the level of security are defined in the settings file, `workstation.properties`, that is located in a folder named `conf` within the installation folder. Changes to values take effect on restarting IUCLID 5. The security features are described below.

The settings are shown below as they appear in the settings file that is supplied with the installation of IUCLID 5. The values are shown set to the hard-coded defaults and commented out. If a line is commented out, the hard-coded default value is used. A value of zero (0) disables a feature.

```
# The minimum length for a new password
# password.min.length=6
# The minimum number of character sets used in the password
# password.min.charsets=2
# If a secure question system is enabled
# password.use.secure.question=true
```

In the example shown below, the security features have been disabled.

```
# The minimum length for a new password
  password.min.length=0
# The minimum number of character sets used in the password
  password.min.charsets=0
# If a secure question system is enabled
  password.use.secure.question=0
```

2.3.4.1. Minimum password length

This feature is used to prevent the use of overly weak passwords for user accounts. The password of a user account must contain at least this number of characters. If an attempt is made to create a password with fewer characters, an informative error message is given and the user is presented with an opportunity to try again.

The security policy is applied to passwords only when they are created. Therefore, if the minimum length of passwords is increased, users can still log in using existing passwords, even if they are now considered to be too short. The user-manager can force a user to create a new password by ticking a box for the account in the IUCLID 5 client. The user is then required to create a new password when they next log in.

2.3.4.2. Minimum number of character sets in passwords

This feature is used to prevent the use of overly weak passwords for user accounts. The password of a user account must contain at least one character from all the character sets. The value is an integer from 1 to 4. A value of 1 means only character set 1, a value of 2 means both character sets 1 and 2, etc. The four character sets are: 1 = a lowercase letter [a-z], 2 = an uppercase letter [A-Z], 3 = a digit [0-9], 4 = a non-alphanumeric symbol [!@#$%^&*-_=+].

For example, if the value is 3, a password of "AdkbScfw" is rejected for being too weak, but "AdkbSc37" is accepted because it contains at least one character from sets 1, 2 and 3.

If an attempt is made to create a password that does not comply, an informative error message is given, and the user is presented with an opportunity to try again.

The security policy is applied to passwords only when they are created. Therefore, if the minimum number of character sets allowed within passwords is increased, users can still log in using existing passwords, even if they are now considered to contain too few character sets. The user-manager can force a user to create a new password by ticking a box for the account in the IUCLID 5 client. The user is then required to create a new password when they next log in.

2.3.4.3. Security question

This feature is designed to allow an alternative method of user authentication to the user name/password combination. It can help to reduce the resources required for user management by preventing account blocking due to forgotten passwords. Each user can define their own security question and a secret answer. This is done from the graphical user interface of the client, after the user has logged in. A user can log in by answering their question correctly, instead of supplying the password. The question is answered via a link on the log in page, Forgot your password?. The feature is turned on or off for the whole instance of IUCLID 5 using a value of `true` or `false`.

2.4. Quick guide to installation and configuration - example for system administrators

What follows is an example of a check list of the sequence of actions required to make a fresh installation of IUCLID 5. It assumes that the user has administrator rights to the installation machine, and experience of system administration under Windows.

1. Install the latest update of Java SE 7 (JRE) for your version of Windows, available without charge within the limits of the license, from the site www.java.com.

2. Download the latest one-click installer for PostgreSQL for your version of Windows. It is available without charge, within the limits of the license, from www.postgresql.org/download. Run the installer. If a Windows user *postgres* does not exist already, the installer wizard will create one and ask you to give it a password. Remember the password for subsequent steps.

3. Create a database *login role* (user) named *iuclid5*. Create a database named *iuclid550* under that login role. Remember the values for subsequent steps. A convenient way to do this is using the graphical admin tool *pgAdmin III* that comes with PostgreSQL.

4. Create an installation directory for IUCLID 5 somewhere convenient, for example `C:\Program Files\IUCLID5`.

5. Copy into the installation directory, all the contents of the directory named `workstation` supplied in the zipped archive of the IUCLID 5 download. Do not unzip any of the plugin files.

6. Set the values for the username and password of the PostgreSQL database user (*login role*) as defined above. The values are stored in the file named, `workstation.properties` that is located in a folder named `conf` within the installation folder. The default values are as follows:

```
hibernate.connection.username=iuclid5
hibernate.connection.password=iuclid5
```

7. Set the values for the level of security for user accounts, as described in Section 2.3.4, “Security settings for user accounts”.

8. Start IUCLID 5 by running the executable file `iuclid5.cmd` from the installation directory. If IUCLID 5 does not run first time, check that PostgreSQL is running as a service and that there is a user named *postgres*.

9. When an installation of IUCLID 5 is started for the first time, the wizard *First Steps* is launched. It is designed to help in the set-up of the installation. Go through the steps of the wizard. Detailed help is available via links denoted by a question mark, *?* at the bottom left of the wizard pages.

10. If the installation has been a success, create any links to `iuclid5.cmd` you might require, for example a shortcut from the Desktop. There is an icon in the installation folder that you can use with a shortcut.

Chapter 3. Upgrade

This document describes the process of obtaining an installation of IUCLID 5.5.0 that contains all the data from a previous version. The details of how to proceed depend on the version being upgraded. There is a chapter specific to each scenario. To see the current version of IUCLID 5, log-in to the application, then click *Help* and select *About*.

Before starting the upgrade, it is important to backup the database. Use the built-in Backup functionality of IUCLID 5, and/or the backup functionality of the database. Making only a copy of the file system on which IUCLID 5 is installed is not recommended as a means of backing-up.

3.1. Upgrading from IUCLID 5.4.x to IUCLID 5.5.0

Important

The migration process changes the IUCLID 5 database such that it can no longer be used with previous versions of the IUCLID 5 application. Therefore, if you would like to be able to continue to use a database with the previous version of IUCLID 5, do not run the migration tool on that particular database. Either perform a fresh installation of the new version of IUCLID 5 and transfer the data across to it using Backup/Restore, or perform the upgrade and migration on a duplicate of the old database. If two versions of IUCLID 5 are to be run on the same computer, appropriate database settings must be used to avoid conflicts. These depend on the particular set-up required. The use of custom database settings is described in Section 2.3, “Post-installation configuration”.

The upgrade is carried out in the following sequence:

1. Back-up the database. Use the built-in Back-up functionality of IUCLID 5, and/or the backup function of the database software, for example PostgreSQL.
2. Remove the executable program files for the previous version of IUCLID 5. The existing plugins for IUCLID 5.4.x are compatible with IUCLID 5.5, so they can be retained for use in the new installation. Alternatively, obtain the latest versions from the IUCLID web site.
3. Install the program files for the latest version of IUCLID 5.5 as follows. Unzip the archive that contains the software for the manual installation of IUCLID 5. Create an installation directory for IUCLID 5 somewhere convenient, for example `C:\ Program Files \ IUCLID5`. Copy the directory `workstation` and all its contents into the installation directory.
4. Transfer the required information from the existing configuration files to the versions supplied in the new installation. See Section 2.3, “Post-installation configuration” for more details.

   Note that if the Oracle database is used, the file `workstation.properties` must contain the following entry:

   ```
   hibernate.connection.driver_class=oracle.jdbc.OracleDriver
   ```

   The previous value was:

   ```
   hibernate.connection.driver_class=oracle.jdbc.driver.OracleDriver
   ```
5. If the database is an Oracle database, please note that the driver for Java is no longer supplied with the IUCLID installation package. The correct driver for the combination of Java and Oracle versions in use must be obtained from the Oracle web site and installed in the appropriate folder. For example, for Oracle 11g Release 2 (11.2.0.2.0), the name of the driver is `ojdbc6.jar`.
6. Copy any required plugins over from the old installation to the new one. Alternatively, obtain the latest versions from the IUCLID web site.

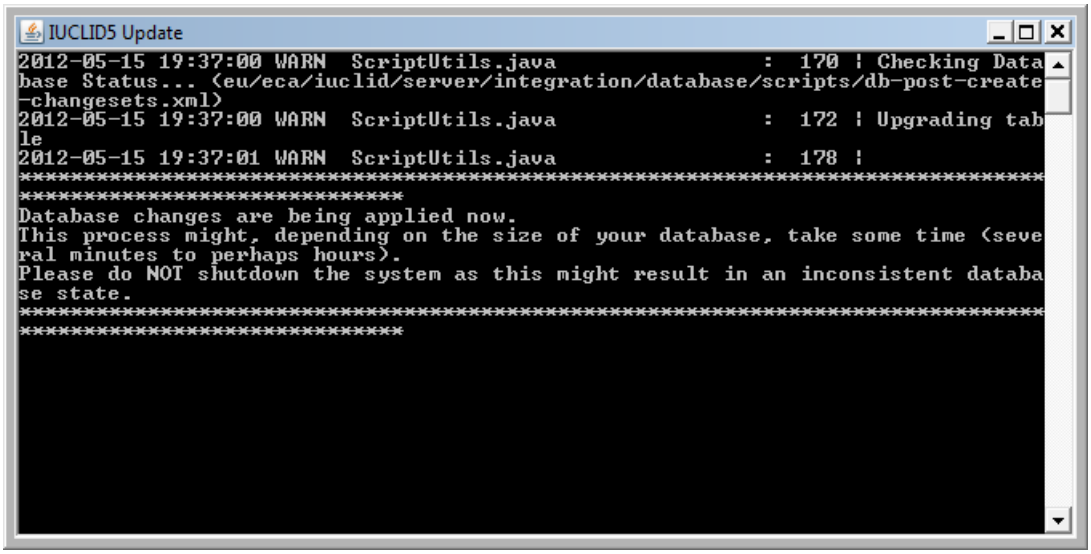
7. A migration process is required to upgrade to IUCLID 5.5. Migrate the database by running the migration tool, as described below. This is a script that is supplied along with the installation package. It makes changes to the database that are required for IUCLID 5.5. IUCLID 5 cannot be started until the migration tool has been run successfully.

8. Once the migration process has been completed successfully, the new version of IUCLID 5 can be started and checked before being entered into production.

3.1.1. The migration tool

The migration tool is a script supplied with the installation package. The file name is `update.bat`. Run the script as you would any other script either from the command line, or by double-clicking on its icon in the Windows file manager. Whilst the migration tool is running, a window is shown for the program *cmd* that contains a terminal to the command line of Windows. A typical example is shown in the screen shot below:

Figure 3.1. Migration tool is running


IUCLID5 Update
2012-05-15 19:37:00 WARN ScriptUtils.java : 170 ! Checking Data
base Status... (eu/eca/iuclid/server/integration/database/scripts/db-post-create
-changesets.xml)
2012-05-15 19:37:00 WARN ScriptUtils.java : 172 ! Upgrading tab
le
2012-05-15 19:37:01 WARN ScriptUtils.java : 178 !
Database changes are being applied now.
This process might, depending on the size of your database, take some time (seve
ral minutes to perhaps hours).
Please do NOT shutdown the system as this might result in an inconsistent databa
se state.

Do not allow anything to happen that might interrupt this process. Do not close the window. When the migration of data has finished, the message *Database update successfully finished* is displayed in the window. The database is then checked automatically and final changes are made. At the end of the process, the final message is *Database is up to date*. The command line window then closes automatically. If the process is interrupted, try starting again from the beginning. If that does not work, restore the original database from a backup, and try again. During the migration process, entries are written to log files named `i5workstation.log` and `iuclidMT.log`. The default path to the log files is `${user.home}/.iuclid5/`. In practice, this leads to a value such as `C:\Documents and Settings\<user name>\.iuclid5` where `<user name>` is the name of the user account in Windows that is used to run IUCLID 5. The file `i5workstation.log` contains statements about the start and end of the migration process. Details of what data is being migrated are included in `iuclidMT.log`. If you need to know what happened during the migration process, check those files first.

3.1.2. Starting IUCLID 5

If the migration tool has run successfully, you can now launch the newly installed IUCLID 5.5 by double-clicking the icon that the installer created on your Desktop, as shown below. It is also possible to launch IUCLID 5 by running the file `iuclid5.cmd` that is included in the installation directory. The initialisation process is not required. All of the data that was present in the upgraded system should be present in the new system. Therefore, it should be possible to log in to any of the user accounts from the previous system.

Figure 3.2. A shortcut to the IUCLID 5 application

3.2. Upgrading from IUCLID 5.2.x/5.3.x to IUCLID 5.5.0

To upgrade from IUCLID versions 5.2.x or 5.3.x, unless the database contains a very large amount of data, it is recommended to use the Backup and Restore features of IUCLID 5 to transfer the data from the old installation to a fresh installation of IUCLID 5.5.0. The Backup and Restore features are described in the IUCLID 5 End-User Manual. Making a fresh installation is described in this manual.

Warning

The built-in Backup functionality of IUCLID 5.3.1 is known to output files in which the user accounts cannot be used on restore. If you wish to use the built-in Backup functionality on data in an installation of IUCLID 5.3.1, first upgrade it to IUCLID 5.3.2. The built-in Backup functionality in IUCLID 5.3.2 does not suffer from this problem.

As an alternative to using Backup and Restore into a fresh installation, it is possible to perform step-wise upgrades in which the database is migrated from IUCLID 5.2.x/5.3.x to 5.4.x to 5.5.0. For example, this method might be required if the amount of data is so large that it makes use of the Backup feature impractical. If you choose the migration method, obtain the installation packages to perform the required upgrades, and then proceed as per the instructions included therein.

Note that the plugins for IUCLID 5.2.x/5.3.x are not compatible with IUCLID 5.5. Therefore, they must not be copied over to the new installation. Compatible versions can be downloaded from the IUCLID web site.

3.3. Upgrading from IUCLID 5.0/5.1.x to IUCLID 5.5.0

To upgrade from 5.0/5.1.x, no migration process is available, and so the method of using Backup then Restore into a fresh installation must be used. In IUCLID 5.0/5.1.x there is no built-in Backup function. Instead, the functionality is provided by a plugin, *Backup Plug-in 5.0.3* that is available on the IUCLID web site under downloads for IUCLID 5.1.1.

Chapter 4. Initialisation of an installation of IUCLID 5

This chapter describes the configuration that is required to create a working IUCLID 5 system from an installation of IUCLID 5 that has an empty database. There are two scenarios: either to create a working installation from scratch, or to load data from a backup that was made using the built-in Backup function of IUCLID 5. During initialisation from scratch, reference substance data and a legal entity are uploaded into the database, and the required user accounts can be created. For initialisation from a backup, make sure that the backup files are accessible from the system on which IUCLID 5 will be initialised. What to do in each scenario is described in the rest of this chapter.

4.1. Starting IUCLID 5

Connect to the application by running the file named `iuclid5.cmd` that is supplied with the installation files. It is convenient to create a shortcut that points to `iuclid5.cmd` and to attach the IUCLID 5 icon that is supplied with the installation files.

Figure 4.1. A shortcut to the IUCLID 5 application

4.2. First steps wizard

When you start IUCLID 5 for the first time, the *First steps* wizard is run automatically. It guides you through the steps required to make a working user account and to upload the data required to use IUCLID 5 in a practical setting. The settings that relate to user accounts can also be changed after having run the wizard, using the features described in the IUCLID 5 End-user Manual.

Important

This wizard allows a single user account to be created, per run. This user is in addition to the *SuperUser* account that comes with the installation. It is essential to have at least one user account in addition to *SuperUser* because *SuperUser* should be used only for the special tasks that only it can carry out. See the IUCLID 5 End-user Manual for more detail.

As part of the First steps wizard, a legal entity must be uploaded into the IUCLID 5 installation in the form of a LEOX file. Therefore, before running this wizard, make sure that a LEOX file for the legal entity of your company or organisation is accessible to your computer. For more information, see the IUCLID 5 End-user Manual.

The First steps wizard provides the option of uploading the following information to your IUCLID 5 installation. For details, see the IUCLID 5 End-user Manual:

- EC Inventory
- Inventory of Reference substances

Although these uploads are optional, it is strongly recommended to do them during the first run of the First steps wizard. To do so, you will need to have the data accessible to your computer whilst running this wizard.

The First steps wizard can be run at any time, but only by the *SuperUser*. This is done from the file menu within IUCLID 5 **Administrative tools** / **Initialise**.

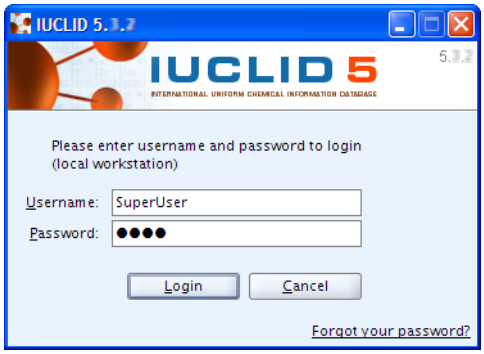
When starting the IUCLID 5 for the first time, the only user available is an administrator named *SuperUser*. Log in as *SuperUser* by entering the following case-sensitive values into the login screen as shown below:

Username: SuperUser

Password: root

Note

Do not click on the link **Forgot your password?** if the *First steps* wizard is being run for the first time on this database. This feature can work only after the wizard has been completed. The use of the feature **Forgot your password?** is explained later in this wizard, at step 3.



The First steps wizard then proceeds. Each page of the wizard is described in a figure below.

Figure 4.2. Step 1 of the First steps wizard - Introduction

The wizard presents some useful information. There are no actions other than to read the information. Click the **Next** button.

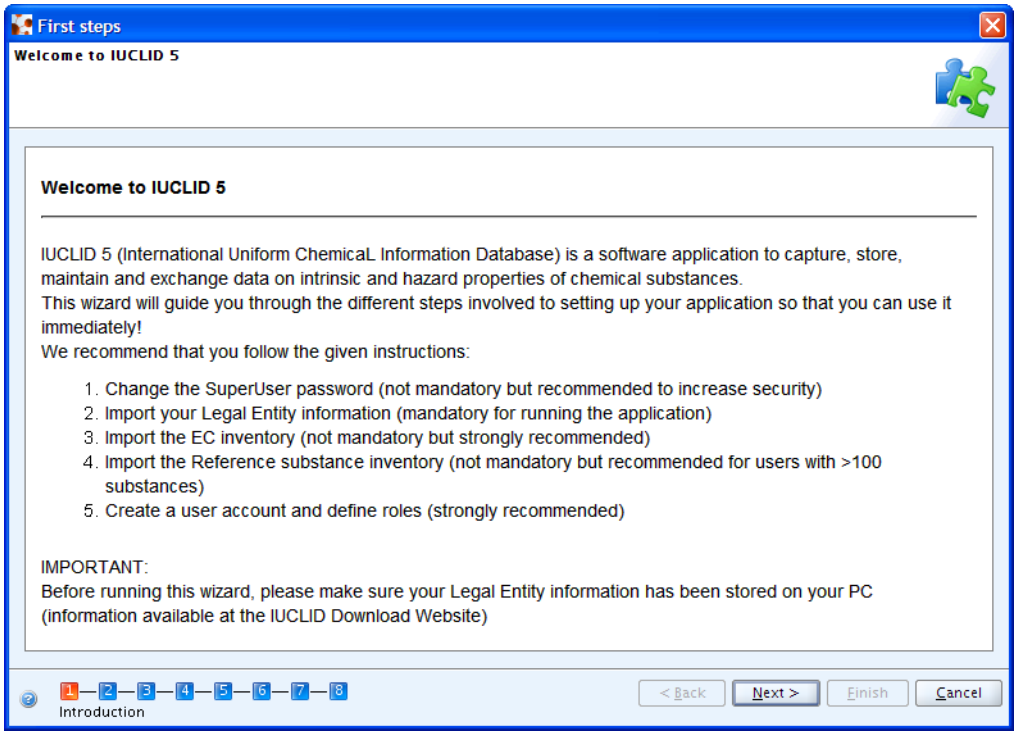

First steps
Welcome to IUCLID 5
Welcome to IUCLID 5
IUCLID 5 (International Uniform ChemicaL Information Database) is a software application to capture, store, maintain and exchange data on intrinsic and hazard properties of chemical substances.
This wizard will guide you through the different steps involved to setting up your application so that you can use it immediately!
We recommend that you follow the given instructions:
1. Change the SuperUser password (not mandatory but recommended to increase security)
2. Import your Legal Entity information (mandatory for running the application)
3. Import the EC inventory (not mandatory but strongly recommended)
4. Import the Reference substance inventory (not mandatory but recommended for users with >100 substances)
5. Create a user account and define roles (strongly recommended)
IMPORTANT:
Before running this wizard, please make sure your Legal Entity information has been stored on your PC (information available at the IUCLID Download Website)
1 2 3 4 5 6 7 8
Introduction
< Back
Next >
Finish
Cancel

Figure 4.3. Step 2 of the First steps wizard - Init mode - New installation

To initialise a new database, select the button `New Installation`as shown below and continue to the next step.

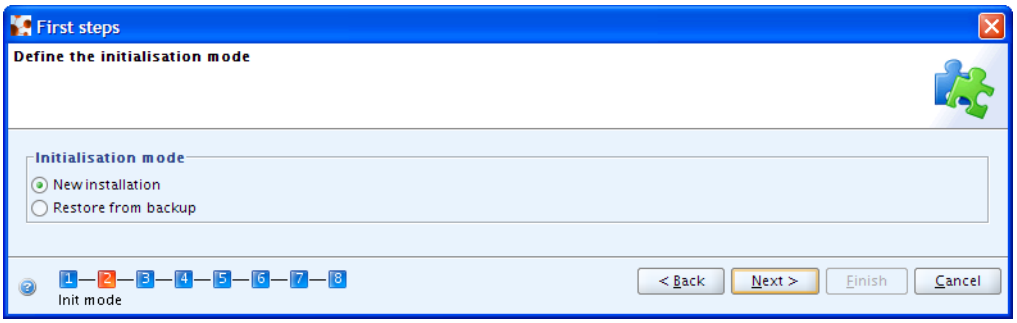
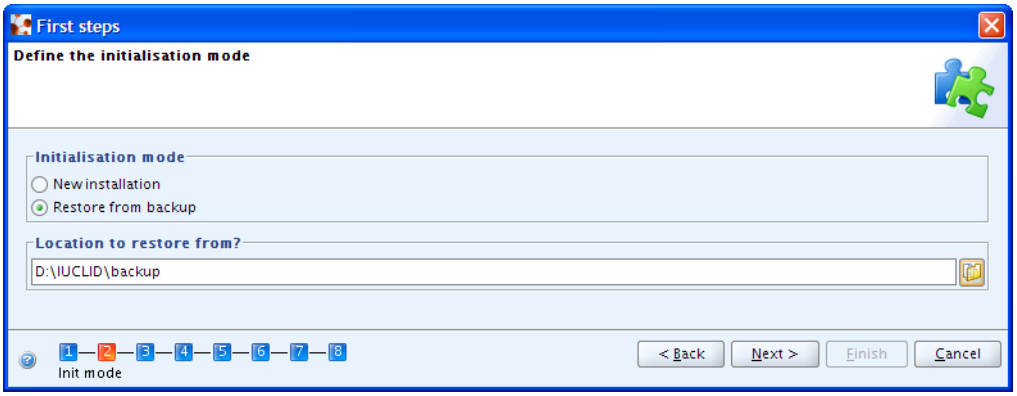


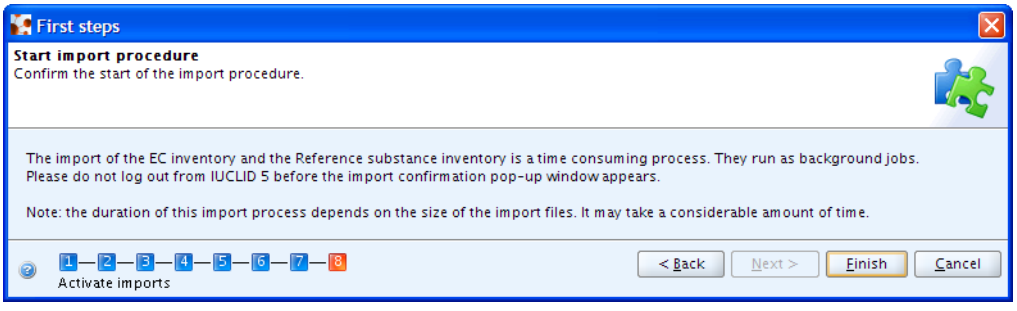
Figure 4.4. Step 2 of the First steps wizard - Init mode - Restore from backup

To restore from a backup of a previous version of IUCLID 5, select the button `Restore from backup` then enter the directory containing the backup files as shown in the example below.



Click **Next**. The wizard jumps to its last step, where the importation of data is started, as shown below.

Figure 4.5. Restoration from a backup - Step 8 - Activate imports


First steps
Start import procedure
Confirm the start of the import procedure.
The import of the EC inventory and the Reference substance inventory is a time consuming process. They run as background jobs.
Please do not log out from IUCLID 5 before the import confirmation pop-up window appears.
Note: the duration of this import process depends on the size of the import files. It may take a considerable amount of time.
1 2 3 4 5 6 7 8
Activate imports
< Back
Next >
Finish
Cancel

The import may take some time. Click *Finish*. When the restoration is complete, the following screen is shown.

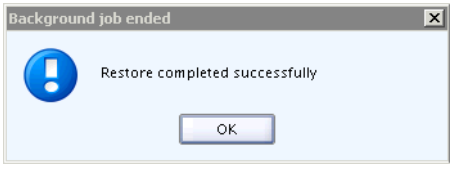
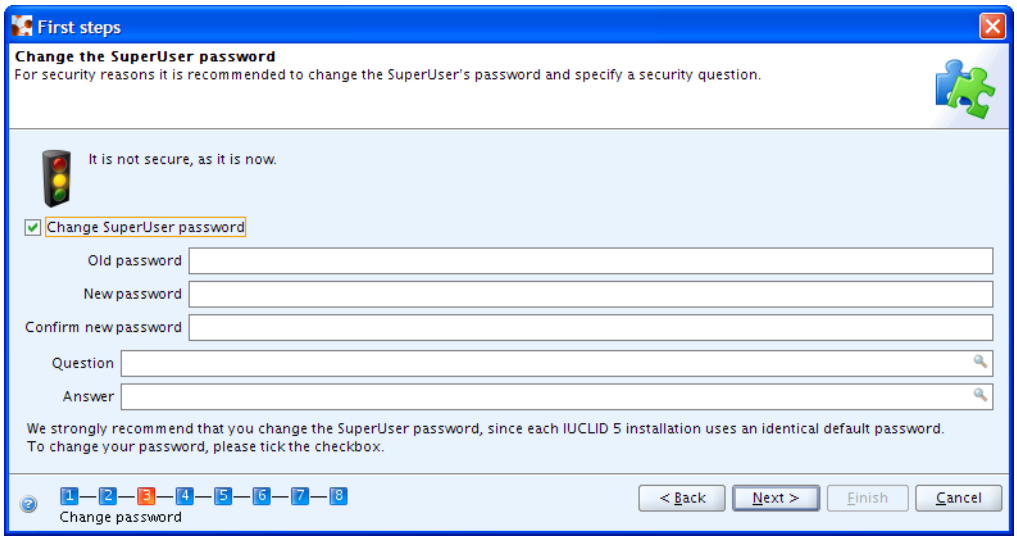


Figure 4.6. Step 3 of the First steps wizard - Change password

If the password for *SuperUser* has never been changed from its default value of *root*, the traffic light in the wizard screen will be yellow. To change the password, check the box `Change SuperUser password` , enter the current password, and then the new password, and then the new password again.

To proceed, click the button **Next**.


First steps
Change the SuperUser password
For security reasons it is recommended to change the SuperUser's password and specify a security question.
It is not secure, as it is now.
Change SuperUser password
Old password
New password
Confirm new password
Question
Answer
We strongly recommend that you change the SuperUser password, since each IUCLID 5 installation uses an identical default password.
To change your password, please tick the checkbox.
1 2 3 4 5 6 7 8
Change password
< Back
Next >
Finish
Cancel

Tip

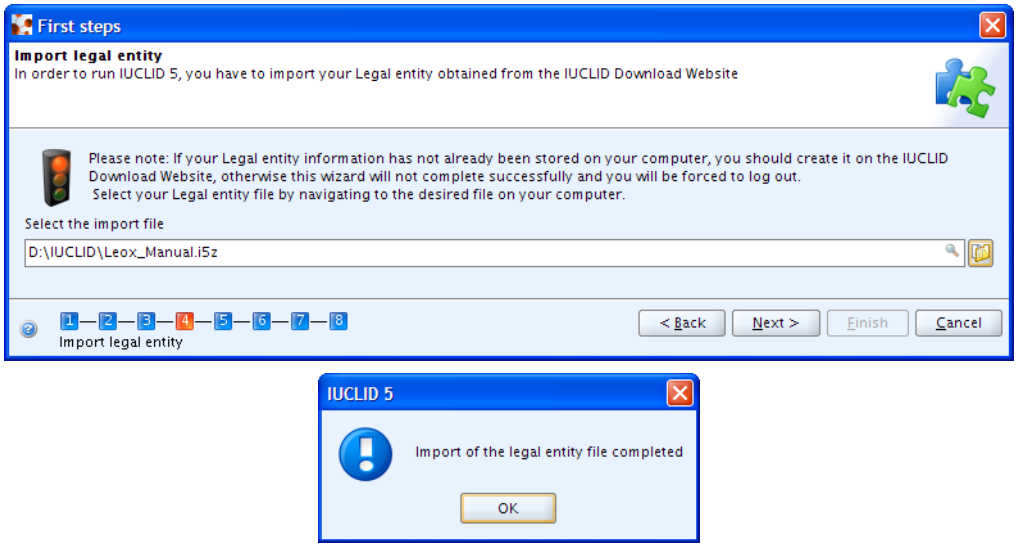
IUCLID 5 has a feature that can check the strength of passwords. If the feature is turned on, and the password you enter is considered to be too weak, an error message is displayed that explains what a password must contain. If that happens, read the error message carefully then create a password that satisfies the criteria. For example, the default settings require the password to be at least 6 characters in length, and to contain at least one uppercase letter, and one lowercase letter. The policy for the SuperUser is the same as that for all users. The password policy is set by editing a settings file within the installation files of IUCLID 5. This is documented in the relevant installation manual for your instance of IUCLID 5. Existing passwords can still be used to log in, even if they do not conform to the current policy. When a password is created, it must conform to the current password policy.

Tip

IUCLID 5 has a feature that allows a user to log in by answering a security question, instead of providing the password for the account. Users define their own questions and answers from within their own accounts. However, the SuperUser is a special case, because the question and answer can be defined before logging in for the first time. The question and answer are entered into the fields shown above in step 3 of the wizard. To use the feature to log in, a user clicks on the link **Forgot your password?** which is situated at the bottom right of the login page.

Figure 4.7. Step 4 of the First steps wizard - Import Legal Entity

To import a Legal entity (see the IUCLID 5 End-user Manual) select its LEOX file by browsing to the file. The browsing is accessed by clicking on the folder icon to the right of the field Select the import file. Click the **Next** button. The Legal entity is imported immediately.


First steps
Import legal entity
In order to run IUCLID 5, you have to import your Legal entity obtained from the IUCLID Download Website
Please note: If your Legal entity information has not already been stored on your computer, you should create it on the IUCLID Download Website, otherwise this wizard will not complete successfully and you will be forced to log out.
Select your Legal entity file by navigating to the desired file on your computer.
Select the import file
D:\IUCLID\Leox_Manual.i5z
1 2 3 4 5 6 7 8
Import legal entity
< Back
Next >
Finish
Cancel
IUCLID 5
Import of the legal entity file completed
OK

Important

You must import at least one Legal entity in order to succeed with this wizard. If you have no Legal entity in the IUCLID 5 system, the traffic light in the wizard screen will be red. The First steps wizard will be automatically launched when you log in to IUCLID 5 until a Legal entity has been successfully imported.

Figure 4.8. Step 5 of the First steps wizard - Import EC Inventory

EC inventory import - To import the EC inventory, select the file for the EC inventory (see the IUCLID 5 End-user Manual). The EC Inventory will not be imported immediately. The import will start at the end of the First steps wizard. Depending on your machine speed and the size of the inventory, this import can take some time, e.g. up to half an hour.

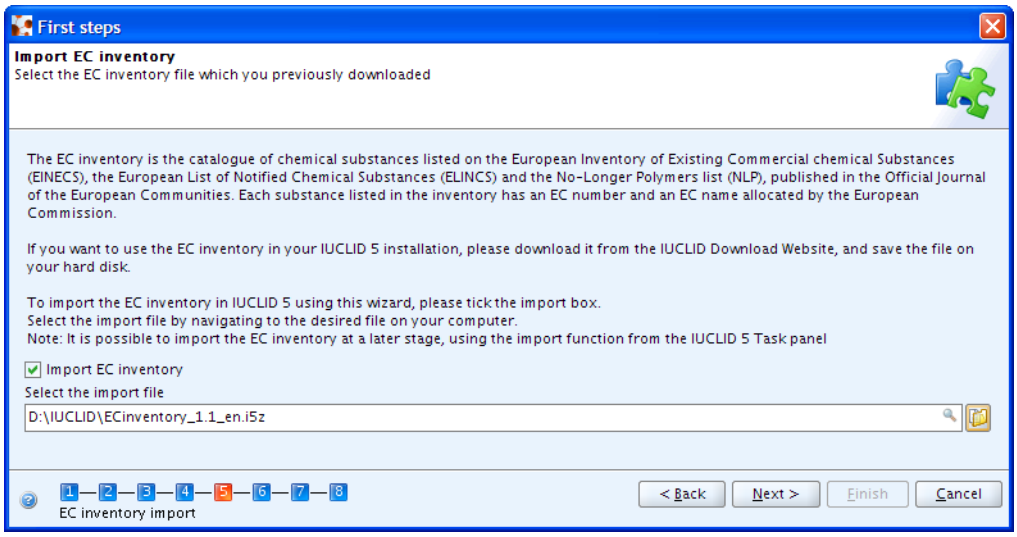
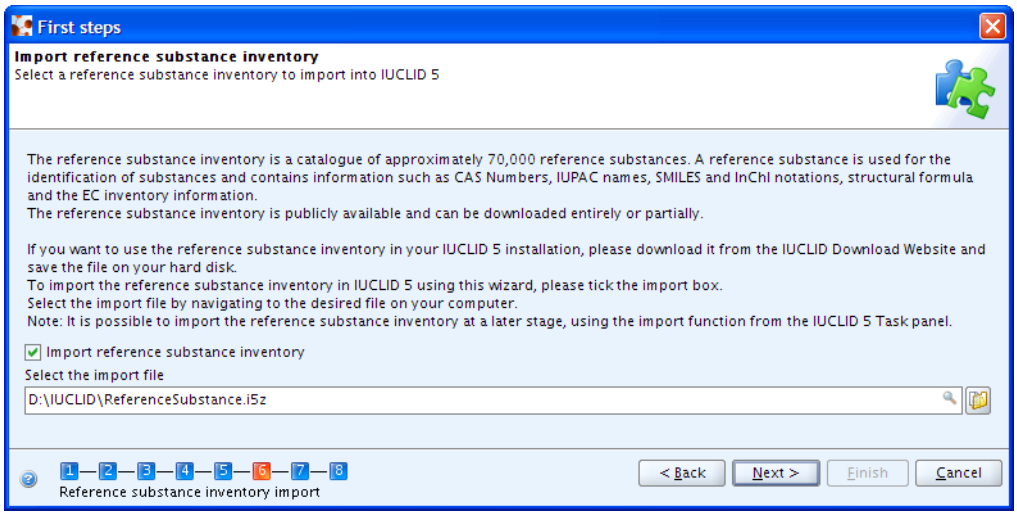

First steps
Import EC inventory
Select the EC inventory file which you previously downloaded
The EC inventory is the catalogue of chemical substances listed on the European Inventory of Existing Commercial chemical Substances (EINECS), the European List of Notified Chemical Substances (ELINCS) and the No-Longer Polymers list (NLP), published in the Official Journal of the European Communities. Each substance listed in the inventory has an EC number and an EC name allocated by the European Commission.
If you want to use the EC inventory in your IUCLID 5 installation, please download it from the IUCLID Download Website, and save the file on your hard disk.
To import the EC inventory in IUCLID 5 using this wizard, please tick the import box.
Select the import file by navigating to the desired file on your computer.
Note: It is possible to import the EC inventory at a later stage, using the import function from the IUCLID 5 Task panel
Import EC inventory
Select the import file
D:\IUCLID\ECinventory_1.1_en.i5z
1 2 3 4 5 6 7 8
EC inventory import
< Back
Next >
Finish
Cancel

Figure 4.9. Step 6 of the First steps wizard - Import reference substance inventory

Reference substance inventory import - Select the file for the Reference substance inventory (see the IUCLID 5 End-user Manual). The Reference substance inventory will not be imported immediately. The import will start at the end of the first steps wizard together with the EC Inventory import. Depending on your machine speed and the size of the inventory, this bulk operation may take a long time. The import of the Reference substance inventory itself can take **up to several hours**.

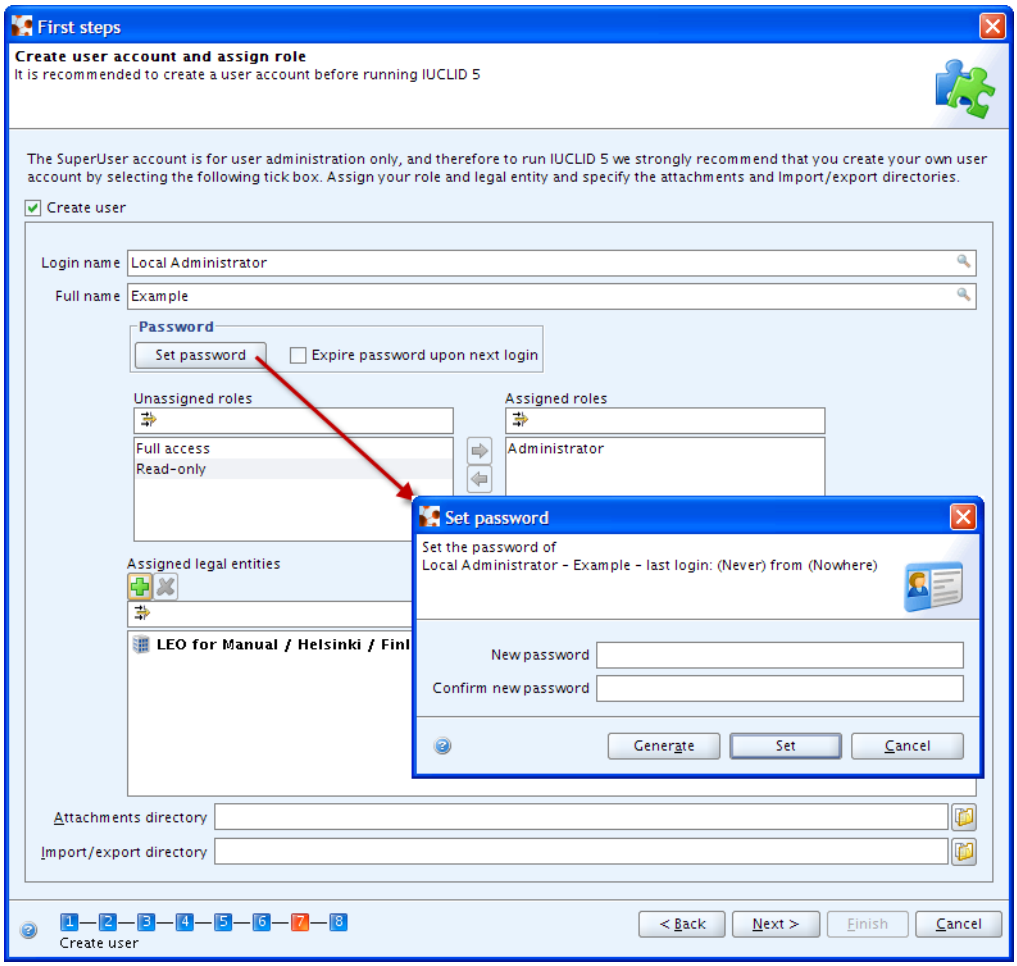

First steps
Import reference substance inventory
Select a reference substance inventory to import into IUCLID 5
The reference substance inventory is a catalogue of approximately 70,000 reference substances. A reference substance is used for the identification of substances and contains information such as CAS Numbers, IUPAC names, SMILES and InChI notations, structural formula and the EC inventory information.
The reference substance inventory is publicly available and can be downloaded entirely or partially.
If you want to use the reference substance inventory in your IUCLID 5 installation, please download it from the IUCLID Download Website and save the file on your hard disk.
To import the reference substance inventory in IUCLID 5 using this wizard, please tick the import box.
Select the import file by navigating to the desired file on your computer.
Note: It is possible to import the reference substance inventory at a later stage, using the import function from the IUCLID 5 Task panel.
Import reference substance inventory
Select the import file
D:\IUCLID\ReferenceSubstance.i5z
1 2 3 4 5 6 7 8
Reference substance inventory import
< Back
Next >
Finish
Cancel

Tip

Time and IT resources can be saved by importing into IUCLID 5 only the Reference substances you need. Various different sizes of Reference substance inventory can be downloaded from the IUCLID web site. There is a *full set,* a *reduced list*, and a function that allows you to create your own inventory using common identifiers as selection criteria, such as EC Number, and IUPAC name. Before importing the *full set*, consider carefully whether it is really necessary. Reference substances that are not imported during the initialisation process can be imported later. A simple compromise is to start with the *reduced list*.

Figure 4.10. Step 7 of the First steps wizard - Create user account and assign role

Create a new user account and define its user access rights by assigning it a role. It is essential to create a new user because general working within IUCLID 5 with the SuperUser is not supported. Only one user can be created per run of the First steps wizard.


First steps
Create user account and assign role
It is recommended to create a user account before running IUCLID 5
The SuperUser account is for user administration only, and therefore to run IUCLID 5 we strongly recommend that you create your own user account by selecting the following tick box. Assign your role and legal entity and specify the attachments and Import/export directories.
Create user
Login name
Local Administrator
Full name
Example
Password
Set password
Expire password upon next login
Unassigned roles
Full access
Read-only
Assigned roles
Administrator
Assigned legal entities
LEO for Manual / Helsinki / Finl
Set password
Set the password of
Local Administrator - Example - last login: (Never) from (Nowhere)
New password
Confirm new password
Generate
Set
Cancel
Attachments directory
Import/export directory
1 2 3 4 5 6 7 8
Create user
< Back
Next >
Finish
Cancel

- Select the checkbox `Create user`.

  Fill in all the fields. The user needs a `Login name` for identification during login. The `Full name` is used for proper user identification. The `Assigned role` is needed to administrate the access permissions. In a newly installed IUCLID 5, the roles *Administrator*, *Full access* and *Read-only* are provided by default.

- Enter a `Login name`, as it should be used for identification during login, and the `Full name` used for proper user identification.

- Click *Set password* to define a password.

Tip

IUCLID 5 has a feature that can check the strength of passwords. If the feature is turned on, and the password you enter is considered to be too weak, an error message is displayed that explains what a password must contain. If that happens, read the error message carefully then create a password that satisfies the criteria. For example, the default settings require the password to be at least 6 characters in length, and to contain at least one uppercase letter, and one lowercase letter. The policy for the SuperUser is the same as that for all users. The password policy is set by editing a settings file

within the installation files of IUCLID 5. This is documented in the relevant installation manual for your instance of IUCLID 5. Existing passwords can still be used to log in, even if they do not conform to the current policy. When a password is created, it must conform to the current password policy.

Tip

If you want a use-once password that is reasonably hard to guess and that definitely conforms to the password policy, you can let IUCLID 5 make one for you, by clicking on the button *Generate*. It will be displayed in a new window for you to make a record of it. On closing that window it will be automatically entered into the fields *New password* and *Confirm new password*.

- Ticking the box *Expire password upon next login* forces whoever logs in to the account first to set their own password.

- Click and highlight a role in the list of unassigned roles and assign it to the user by clicking the Right arrow. Assigning a Role is needed to administrate the access permissions (in a newly installed IUCLID 5, the roles *Administrator*, *Full access* and *Read-only* are provided by default).

Tip

It is recommended to create a user with the *Administrator* Role regardless of whether a stand alone or a distributed version of IUCLID 5 is set up. Once a user has been created, the IUCLID 5 administrator (in case of a distributed version) can define different other user(s) and assign different role(s) to them (see the IUCLID 5 End-user Manual).

- Assign a Legal entity (normally the Legal entity imported in the third step of this wizard) by clicking the green plus button and performing a search for the desired Legal entity. In the Query field `Legal entity name`, enter the name of the desired Legal entity or an asterisk (*) as wildcard and click the **Search** button. In the Query results list, click the desired entry and then click the **Assign** button.

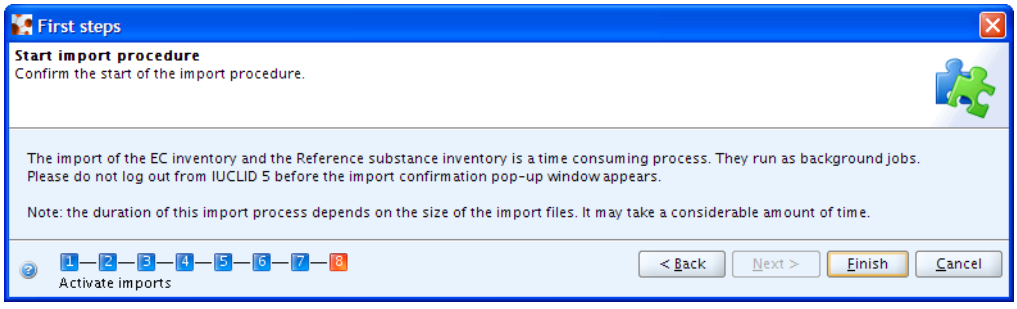
- Optionally, select default attachment and import/export directories. These settings can be changed at a later stage, as described in the IUCLID 5 End-user Manual.

- Click the **Next** button

Figure 4.11. Step 8 of the First steps wizard - Start import procedure

If you have selected an EC Inventory and/or Reference substances inventory file(s) during the wizard steps, you can now run the imports. Click the button **Execute imports**. Note again that these imports can take up to several hours, depending on your machine speed and the amount of data you are importing.

Then click the button **Finish**. If you have launched any imports, you will now have to wait until the imports are completed. Afterwards, you should log out and then log in again as a user for the newly defined account. Remember: general working as SuperUser is not supported.


First steps
Start import procedure
Confirm the start of the import procedure.
The import of the EC inventory and the Reference substance inventory is a time consuming process. They run as background jobs.
Please do not log out from IUCLID 5 before the import confirmation pop-up window appears.
Note: the duration of this import process depends on the size of the import files. It may take a considerable amount of time.
1 2 3 4 5 6 7 8
Activate imports
< Back
Next >
Finish
Cancel

4.3. User management

The installation of IUCLID 5 is now ready for hand-over to whoever will be maintaining the system and whoever will be managing the user accounts. The management of user accounts and their roles is described in the IUCLID 5 User Manual.

Chapter 5. Un-installation of IUCLID 5

The un-installation of IUCLID 5 is a manual process. IUCLID 5 can be un-installed by deleting the files that were copied to the destination machine, and reversing any changes made during the installation process. For more details about the actions that might be required, see the IUCLID FAQ located at the IUCLID web site http://iuclid.eu.